Quantum dynamics of bosons in a double-well potential: Josephson oscillations, self-trapping and ultralong tunneling times

A. N. Salgueiro and A. F. R. de Toledo Piza
Instituto de Física, Universidade de São Paulo, CP 66318 CEP 05389-970, São Paulo, SP, Brazil

G. B. Lemos, R. Drumond and M. C. Nemes
Departamento de Física, Instituto de Ciências Exatas, Universidade Federal de Minas Gerais, CP 702, CEP 30161-970, Belo Horizonte, Minas Gerais, Brazil

M. Weidemüller
Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany

The dynamics of the population imbalance of bosons in a double-well potential is investigated from the point of view of many-body quantum mechanics in the framework of the two-mode model. For small initial population imbalances, coherent superpositions of almost equally spaced energy eigenstates lead to Josephson oscillations. The suppression of tunneling at population imbalance beyond a critical value is related to a high concentration of initial state population in the region of the energy spectrum with quasi-degenerate doublets resulting in imbalance oscillations with a very small amplitude. For unaccessible long times, however, the system recovers the regime of Josephson oscillations.

PACS numbers: 03.75.Lm, 03.65.-w, 05.30.Jp

The understanding of many-body quantum systems from the theoretical and experimental points of view has undergone a considerable development during the past decade. Unifying concepts of several branches of physics are under development, creating an interdisciplinary scenario for the understanding of quantum mechanical paradigms. One of the simplest many-body systems to be realized experimentally and studied theoretically are ultracold bosons in a double-well potential. This system is very rich exhibiting a great variety of quantum phenomena such as interference [1], tunneling/self-trapping [2, 3, 4, 5, 6, 7], entanglement of macroscopic superpositions [8]. Lately this system has been extensively studied, especially after the implementation of several experiments in the area. The usual theoretical approach to weakly interacting Bose-Einstein condensates (BECs) is the mean-field approximation, a nonlinear Gross-Pitaevski equation [3, 9, 10, 11, 12, 13, 14, 15, 16], which has proven very adequate in explaining a wide variety of experiments.

More recently, the dynamics of population distribution between two or more wells of an optical lattice have been experimentally investigated. In particular, Josephson oscillations have been observed in a 1D optical lattice [17, 18] and recently the density distribution of tunneling ^{87}Rb particles is directly observed [2]. In this experiment, initial population differences between the left and right well components are controlled by loading the BEC into an asymmetric double-well potential. The Josephson dynamics is initiated at $t = 0$ by non-adiabatically changing the potential to a symmetric double-well. When the initial population imbalance is below a critical value, the system presents Josephson oscillations between the two sides of the well. However, above this critical value tunneling is not observed. Based on a mean field treatment, this is usually attributed to macroscopic self-trapping. In the present work, we discuss an alternative approach to this system based on exact numerical solutions of the two-mode Bose-Hubbard Hamiltonian [19]:

$$H = -\frac{J}{2}(a_1^\dagger a_2 + a_2^\dagger a_1) + \frac{U}{2}(n_1(n_1-1) + n_2(n_2-1)) + \frac{\delta}{2}(n_1 - n_2) \tag{1}$$

where $a_i^\dagger$ and a_i are, respectively, the creation and annihilation operators of a boson in the i-th site, n_i the occupation number in the i-th site, U is the two-particle on-site interaction, δ is the trap depth difference between the two wells, J is the tunneling matrix element between adjacent sites i,j. which characterizes the strength of the tunneling term.

In this Letter we present a different view on the experimental non-observation of tunneling for initial population imbalances larger than a critical value z_c. The dynamics of the system is related to the properties of the energy spectrum and to the distribution of populations and coherences of the initial wave-function. It is important to notice that this model displays many-body features such as highly correlated many-body eigenstates. In these eigenstates the number of atoms in each well is not defined but features correlated fluctuations. According to the present model, for certain range of the parameter J/U the spectrum of the many-body Hamiltonian presents a region with nearly degenerate doublets, as shown in Ref. [3] and Fig. 1. For sufficiently large initial population imbalance, mainly doublets will participate in the tunneling process. The tunneling period will be approximately

given by $t \sim \hbar/\Delta E_{doublets}$ where $\Delta E_{\mathrm{doublet}}$ stands for the small inner energy difference of the doublets. This energy splitting as $\Delta E_{\mathrm{doublet}}/U = [2N(J/U)^N]/(N-1)!$ (calculated via the doorway method of Ref [23]). For example, for $N = 100$ particles, $J/U = 0.333$, $\Delta E_{\mathrm{doublet}}/U \sim 3.76 \times 10^{-202} \rightarrow 0$. This energy splitting is usually very small and hence will result in periods which are much longer than the time window of the experiments. In the experimental situation of Ref. [2], only much shorter times are observed which is far from the time the tunneling actually happens, giving the idea of "self-trapping". This short time regime is characterized by oscillations with small amplitude which are related to the small coherence between the two pairs of adjacent quasi-degenerate doublets of the spectrum. For this case, the oscillation period is given by the inverse of the energy splitting of adjacent quasi-degenerate doublet, e.g., $t = \hbar/\Delta E$, with $\Delta E/U \simeq (N-1)$. For this reason, the interpretation of the non-observation of tunneling in the model is radically different from the one coming from the Gross-Pitaevski equation, attributed to the non linearity of the mean-field approach [5]. The same analysis can be extended to the improved two-mode model developed in Ref. [13].

To illustrate our ideas, we study a hundred particles in a double-well potential. The upper graphic in Fig. 1 shows the energy spectrum for the symmetric case at $J/U = 3.333$ and $N = 100$, which corresponds to the parameter $\Lambda \equiv \frac{NU}{2J} = 15$ used in the experimental situation of Ref. [2]. The spectrum is composed of two regions: one region of almost equidistant energy levels and one region consisting of quasi-degenerate doublets. (see also Ref. [3]). The dynamics of population in these two regions differs vastly. It has been shown in Ref. [11] that the eigenstates of the system confirm the physical pendulum characteristics of the eigenstates. The ground state is a minimum uncertainty wave packet in both number and phase which is centered at the origin. The harmonic-oscillator-like low-lying excited states are the analog of pendulum librations, and the higher-lying cat like states are the analog of pendulum rotor motions, with a clear signature of the quantum separatrix state where the libration and rotation states separate. This separatrix divides the energy spectrum in two regions, with or without quasi-degenerate doublets which can be directly observed in the upper graph of Fig. 1. The existence of these two distinct spectrum regions has a direct consequence for the dynamics.

The tunneling dynamics is characterized by the time evolution of the population imbalance

$$
\begin{aligned}
z(t) &\equiv \langle\psi(t)|(n_2 - n_1)|\psi(t)\rangle/N \\
&= \sum_m z_{mm} + 2\sum_{m<m'} z_{mm'} \cos[\frac{(E_m - E_{m'})t}{\hbar}] \quad (2)
\end{aligned}
$$

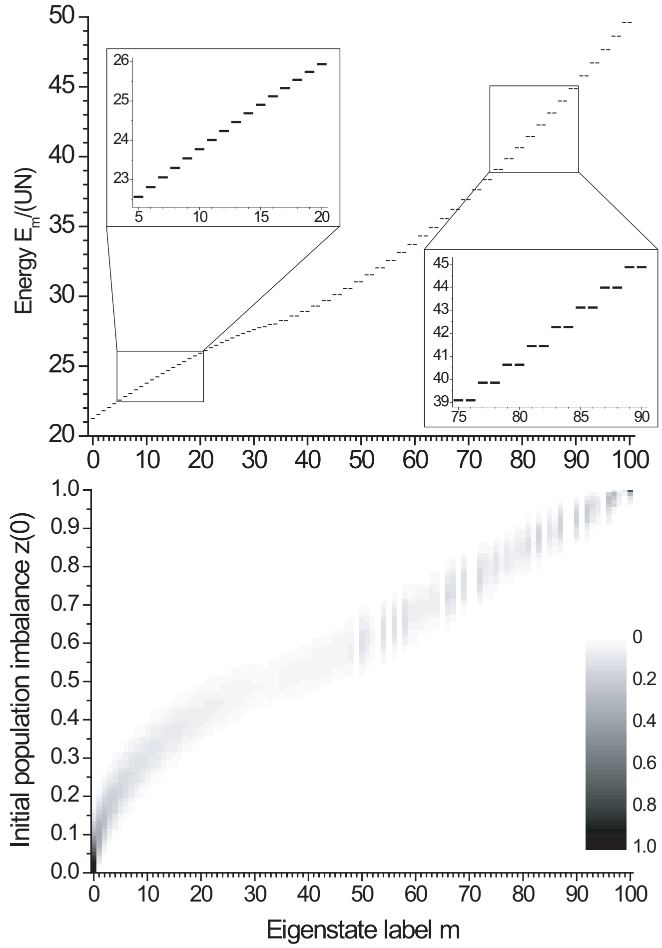

FIG. 1: Upper graph: Hamiltonian energy spectrum for 100 bosons in a symmetric double-well potential for $J/U = 3.333$ corresponding to $\Lambda = 15$. Lower graph: Density plot of the occupation probability of symmetric Hamiltonian eigenstates $|m\rangle$ as a function of the initial population imbalances $z(t = 0)$ for the same parameters as the upper graph. The gray scale gives the population of the corresponding eigenstate. Below a critical value $z_c \approx 0.5$, only states with almost equal energy spacing are populated, while above z_c the quasi-degenerate doublet states are occupied.

where $|\psi(t)\rangle = \sum_m c_m e^{-iE_m t}|m\rangle$ and $z_{mm'} = c_m^* c_{m'}\langle E_m|(\hat{n}_1 - \hat{n}_2)|E_{m'}\rangle/N$, with E_m and $|m\rangle$ being, respectively, the eigenvalues and eigenstates of the hamiltonian in the symmetric case ($\delta = 0$ in Eq. (1)), $c_m = (\langle m|\psi(0)\rangle)$ and $|\psi(0)\rangle$ is the initial many-body wavefunction. Following the experimental approach of Ref. [2] the initial condition is then prepared by non-adiabatically transferring the the ground state of an asymmetric double-well potential $\delta \neq 0$ to the symmetric double-well. This corresponds to a projection of the ground state wavefunction for the asymmetric Hamiltonian $\delta \neq 0$ to the basis $|m\rangle$. The initial state thus critically depends on the value of the parameter δ which is characterized by the initial population imbalance $z(0)$.

Two regions of the energy spectrum can be accessed choosing appropriate initial conditions for the many-body wavefunction of the system. In the lower graph of Fig. 1 the occupation probability $|c_m|^2$ of the eigenstates $|m\rangle$ as a function of the initial population imbalance $z(0)$ is depicted. For small $z(0)$ only the lowest few energy eigenstates are populated. The spread of the distribution of populated states increases as $z(0)$ increases, but for $z(0)$ below a critical value $z_c \approx 0.5$ only energy eigenstates with nearly equal energy splitting are occupied (see upper graph in figure 1). As follows from Eq. 2, coherences between these states will lead to a macroscopic oscillation of the population imbalance at a frequency given by the energy splitting. For larger values $z(0) > z_c$ this scenario changes and only doublet states are occupied. These states are characterized by superposition states in the basis of states confined to the left and right side of the double. As these two states are almost degenerate, coherences among them do not contribute to the oscillatory term in Eq. 2.

The dynamical behavior of the system $z(t)$ crucially depends on the competition of the two ingredients of $z_{n,m}$, the correlation matrix of the initial state in the basis of the eigenstates of the symmetric hamiltonian $c_m^* c_n$ and the correlation matrix of the observable, the population imbalance in the basis of the eigenstates of the symmetric hamiltonian $\langle E_m|(n_1 - n_2)|E_n\rangle$. The second term is responsible for the suppression of the population oscillations of the first term. As the occupied eigenstates are almost equally spaced for $z(0) < z_c$, the population imbalance $z(t)$ oscillates around zero at a fundamental oscillation frequency given by the mean energy spacing of the occupied states, which is given by the plasma frequency $\omega_p = 2J\sqrt{1+\Lambda}$, with $\Lambda = (UN/2J)$ [5]. This behavior constitutes the regime of Josephson oscillations as shown by the left graph of the upper curves in Fig. 2. Small deviations from equal energy spacing lead to a damping of the oscillation on a time scale inversely proportional to the number of occupied states and the corresponding differences in energy splitting. The oscillations undergo revivals on time scales given by the inverse of the frequency difference of adjacent eigenstates. The revivals can be seen in the right graph of the upper curves in Fig. 2. For larger values of $z(0) > z_c(0)$, where doublet states are occupied with negligible coherences between adjacent doublet, one observes two different time scales, characterized by a regime with small or large oscillation amplitude. For the smaller time scales, the population imbalance is locked to its initial value with small residual oscillations as shown by the left graph of the lower curves in Fig. 2. The frequency of these small oscillations is determined by the inverse of the energy splitting of two quasi-degenerate doublets, i.e. $\Delta E \simeq NU$. The latter regime is commonly the "Self-Trapping" regime observed in Ref.[2]. It should however be noted, that on larger time scales $T \simeq \hbar/\Delta E_{\mathrm{doublet}}$, which are far beyond experimental observation, the atoms still undergo collective tunneling resulting in oscillatory behavior of the population imbalance around zero, since the initial condition guarantees a high occupation of the quasi-degenerate doublets, as one can see in the lower graph of figure 1.

The time average of the population imbalance $\overline{z(t)}$ over 50 plasma periods $(2\pi/\omega_p)$ is shown in Fig 3 for different values of Λ as a function of the initial population imbalance $z(0)$ and gives the critical value z_c for which the system crosses from the Josephson regime (oscillations around $z = 0$) to a self-trapping regime. From Fig 3 one sees that as the parameter Λ decreases, the critical value z_c increases for a fixed number of particles N. This can be understood in terms of the structure of the symmetric hamiltonian energy spectrum. The number of quasi-degenerate doublets increases as the tunneling parameter J/U decreases (Λ increases). As a consequence, the quasi-degenerate doublets have lower energies which can be accessed by lower values of z_c, providing an increase of the self-trapping region, since the region of high distribution of the initial population imbalance in the quasi-degenerate doublets also increases. The critical values z_c of Fig 3 follow very well the semiclassical prediction $z_c \simeq 2\sqrt{1+\Lambda}/\Lambda$.

In spite of the obvious advantages of an exact approach, there are several limitations to the model. The two mode assumption is an approximation to the real situation. More restrictive, however, is the hypothesis that the coefficients J and U remain constant in time. This approximation is only valid when the many-body interactions produce small modifications on the ground state properties of the individual wells. This is true if the on-site interaction energy is much smaller than the level spacing of the external trap (see [3]). In this case the number of atoms $N \ll \sqrt{\frac{\pi}{2}}\frac{r_0}{|a|}$, where a is the scattering length and r_0 is the position uncertainty in a harmonic oscillator ground state. In the experiment with ^{87}Rb of ref. [2, 22], $N \ll 200$. However, qualitative behavior is still observed.

We have investigated the dynamics of the imbalance population of bosons in a double-well potential from the point of view of a many-body Hamiltonian in the framework of the two-mode model. Although the model is not realistic enough for large numbers of particles ($N \geq 200$), it points out a completely different explanation for the suppression of tunneling. There are no nonlinearities in this system and therefore the tunneling process is explained solely in terms of initial conditions and spectral properties of the many-body Hamiltonian. In this context, the spectrum is divided in two regions, one of them consisting of quasi-degenerate doublets. When the initial condition is small such that $z(0) < z_c$, the occupation probability is larger in the lower part of the energy spectrum with quasi-equidistant levels, contributing with large oscillation amplitude with a plasma frequency ω_p. When the initial population imbalance is large enough

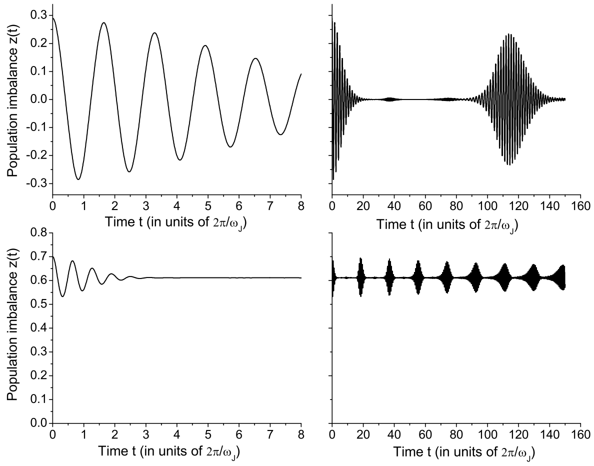

FIG. 2: Time evolution of the population imbalance 100 particles for $J/U = 3.333$ and initial conditions $z(0) = 0.3$ (upper graph) and $z(0) = 0.7$ (lower graph).

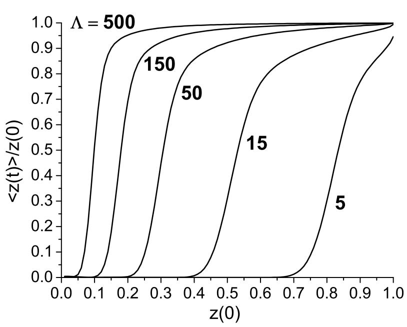

FIG. 3: Time average of $\overline{z(t)}/z(0)$ over 50 plasma periods as a function of the initial population imbalance $(z(0))$ for 100 particles. Josephson oscillations result in $\overline{z(t)} = 0$ while $\overline{z(t)} \neq 0$ indicates the regime of suppressed tunneling. The parameter $\Lambda = NU/2J$ determines the critical population imbalance separating these two regimes.

$z(0) > z_c$ only the quasi-degenerate doublets are appreciably occupied. For small time range, the system oscillates with a very small amplitude, whose oscillation period is given $t \simeq \hbar/(U(N-1))$. However, for longer times, the system recovers the Josephson oscillation behavior, with a large amplitude and oscillatory period of $t \simeq \Delta E_{\text{doublet}}/U = (\frac{2N(J/U)^N \hbar}{(N-1)!})$ .In this case the tunneling time given for a large number of particles is beyond observational possibility. Hence, the "self-trapping" observed in the experiment of ref.[2] is related to the behavior of the imbalance population for short time. The same analysis can be extended to the improved two-mode model of ref[13], which includes the terms reflecting the physics of the transfer of atoms from one well to the other due to collision excluded from the two-mode model, since the energy spectrum of the improved model has the same structure as the two-mode model, i.e. it is also divided into a region with and without quasi-degenerate doublets. Therefore, the same qualitative physical picture would result by this extension of the present model.

A.N.S. is supported by FAPESP and acknowledges M. Oberthaler for discussions. M.C.N and R.D. thank CNPq for financial support. G.B.L thanks CAPES for financial support. M.W acknowledges financial support by DFG under WE $2661/1-3$ and DAAD in the framework of the PROBRAL programme.

[1] M.R. Andrews *et al.*, Science **275**, 637 (1997).
[2] Michael Albiez *et al.*, Phys. Rev. Lett. **95**, 010402 (2005).
[3] G. Milburn *et al*, Phys. Rev. **A 55**, 4318 (1997).
[4] S. Raghavan *et al*, Phys. Rev. **A 59**, 620 (1999);
[5] A. Smerzi *et al*, Phys. Rev. Lett. **79**, 4950 (1997).
[6] J. Ruostekoski and D. Walls, Phys Rev. **A 58**, R50 (1998).
[7] F. Meier and W. Zwerger, Phys. Rev. **A 64**, 033610 (2001).
[8] A. Micheli *et al*, Phys. Rev. **A 67**, 013607 (2003).
[9] A.P. Hines *et al*, Phys. Rev. **A 67** 013609 (2003).
[10] A.J. Leggett, Rev. Mod. Phys, **73**, 307 (2001).
[11] L.D. Carr *et al*, Phys. Rev **A 62**, 063610 (2000); L.D. Carr *et al*, Phys. Rev **A 62**, 063611 (2000); K.W. Mahmud *et al*, Phys. Rev. **A 66**, 063607 (2002).
[12] Khan W. Mahmud *et al*, Phys. Rev. **A 71**, 023615 (2005).
[13] D. Ananikian and T. Bergeman, Phys. Rev **A 73**, 013604 (2006).
[14] A.F.R. de Toledo Piza, Brazilian Journal of Physics, **34 n3B**, 1102 (2004).
[15] J.R. Anglin *et al*, Phys. Rev. **A 64**, 063605 (2001).
[16] H.-Q. Zhou *et al*, J. Phys. A: Math. Gen. **36**, L113 (2003); Feng Pan and J.P. Draayer, cond-mat/0410423 (attractive on site interaction).
[17] F. Cataliotti *et al*, Science **293**, 843 (2001).
[18] B. P. Anderson and M. A. Kasevich, Science **282**, 1686 (1998).
[19] M.P.A. Fisher *et al.*, Phys. Rev. **B 40**, 546 (1989).
[20] J. Schwinger, *Quantum Theory of Angular Momentum*, L. Biedenharn and H. Van Dam, Eds., Academic Press, New York (1965).
[21] A.N. Salgueiro *et al*, Physica **A 290**, 4 (2001).
[22] M. Albiez, "Observation of nonlinear tunneling of a Bose-Einstein condensate in a single Josephson junction" , PhD dissertation thesis presented at the Ruperto-Carola University of Heidelberg, Germany (2005).
[23] A.N. Salgueiro *et al*, cond-mat/0510120.